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Initial Conditions for a Universe*

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Abstract

In physical theories, boundary or initial conditions play the role of selecting special situations which can be described by a theory with its general laws. Cosmology has long been suspected to be different in that its fundamental theory should explain the fact that we can observe only one particular realization. This is not realized, however, in the classical formulation and in its conventional quantization; the situation is even worse due to the singularity problem. In recent years, a new formulation of quantum cosmology has been developed which is based on quantum geometry, a candidate for a theory of quantum gravity. Here, the dynamical law and initial conditions turn out to be linked intimately, in combination with a solution of the singularity problem.

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By design, physical theories provide a framework to deal with a large class of situations in such a way that a variety of different phenomena can be seen to have their origin in a small number of basic physical concepts. As an example, Maxwell theory links seemingly unrelated observations in optics and electricity as properties of the electromagnetic field. Usually, a theory also contains rules how to specify boundary or initial conditions in order to select a special class of systems within a vast range of possibilities which can be realized, e.g., in a certain experimental setup. The particular choice of those conditions, however, is left open by the theory.

In cosmology, the theory of the universe as a whole, the situation has long been expected to be different: as observers, we have access only to one particular realization of the universe, and its initial conditions cannot be changed. This should be reflected in the fundamental theory of the cosmos; initial conditions for a universe should be part of the theory, rather than the choice of a theorist.

In classical cosmology as described by general relativity, however, the situation is different, even worse thanks to the singularity problem according to which a universe like our own has to start with a "big bang" singularity. At such a point the theory breaks down and initial conditions cannot be imposed there.

To illustrate this, we can look at the simplest case which is an isotropic universe with flat space. Its dynamical law, derived from Einstein's field equations, is the Friedmann equation

$$\left(\frac{\dot{a}}{a}\right)^2 = \tfrac{16\pi}{3} G\rho(a) \tag{1}$$

which describes the evolution of the radius $a(t)$ of the universe as a function of time. If we know the gravitational constant G and the matter content which enters via the energy density $\rho(a)$, we can determine the evolution. For a particular realization, we have to choose initial values $a(t_0)$ and values of possible matter fields at some initial time t_0.

Ideally, t_0 would be the "creation time" of the universe where the initial conditions are either chosen or, hopefully, predicted by the theory. However, in classical cosmology the initial time represents a singularity where the theory breaks down. For instance, if we choose the matter content to be pure radiation the energy density $\rho(a)$ is proportional to a^{-4} and any solution of the Friedmann equation has the form $a(t) \propto \sqrt{t - t_0}$. At t_0 the radius of the universe vanishes which implies that energy densities or tidal forces are infinite and the evolution as described by the Friedmann equation breaks down. Those are the unmistakable signs of a singularity, which can be reached in a finite amount of an observer's time but presents a boundary to what the theory can tell us. There is no way to tell what happens beyond the singularity or if there even is any "beyond the singularity".

The cosmological singularity is often viewed as the point of creation of the cosmos via a big bang. But initial conditions cannot be imposed there since the evolution equation (1) would give us an infinite time derivative of a. Instead, we have to choose another time where the system is not singular and impose initial conditions there which then are completely arbitrary.

The singularity presents a problem by itself which is often hoped to be cured by quan-

tization. In fact there is reason to be optimistic since also in quantum mechanics a classical problem, the instability of the Hydrogen atom, is solved by the presence of a finite ground state energy $E_0 = -\frac{1}{2} m_e e^4/\hbar^2$. Up to inessential constant factors this is the only non-relativistic energy value which can be obtained from fundamental constants just for dimensional reasons. Without $\hbar$, there would simply not be any natural value for a possible lowest energy. Moreover, one can see that it is important to quantize because $\hbar$ appears in the denominator. Thus, in the classical limit $\hbar \to 0$ the ground state energy diverges and we return to instability. As we know, there are also other effects of E_0, most importantly the discreteness of the energy spectrum.

For gravity, we can use a similar argument: Its fundamental parameter is the gravitational constant G which, together with $\hbar$ gives us a natural length, the Planck length $l_{\mathrm{P}} = \sqrt{G\hbar} \approx 10^{-33}$cm. If the Hydrogen atom is any indication, we can expect to have a smallest length in a quantum theory of gravity which would lead to a very different behavior close to the cosmological singularity. We do not notice this length scale in experiments because it is so tiny, but it should have important implications in physical situations which involve small scales. In the classical limit $\hbar \to 0$, the minimal length would approach zero and we can expect to see the singularity problem arise in this way. Furthermore, we can also anticipate that the presence of l_{P} implies a discreteness of space or length spectra. The explicit form of such a spectrum can only be derived from a detailed theory, but its presence can be expected purely on dimensional grounds.

Thus, it seems worthwhile to quantize cosmology; but it is not expected to be straightforward: since classical cosmology is part of general relativity, we need at least a part of a quantum theory of gravity. An approach tailored to simple models as the one we discussed before, is the Wheeler–DeWitt quantization. We replace $\dot{a}$ in the Friedmann equation by the momentum $p_a = 3a\dot{a}/8\pi G$ and use the familiar quantum mechanical procedure to replace p_a with the operator $\hat{p}_a = -i\hbar \mathrm{d}/\mathrm{d}a$ acting on a wave function $\psi(a)$. Choosing an ordering of operators, we obtain the Wheeler–DeWitt equation

$$-\frac{1}{6} l_{\mathrm{P}}^4 a^{-1} \frac{\mathrm{d}}{\mathrm{d}a} a^{-1} \frac{\mathrm{d}}{\mathrm{d}a} a\psi = 8\pi G \hat{H}(a)\psi \tag{2}$$

where $\hat{H}(a)$ is a matter Hamiltonian which we do not need to specify for our purposes. This equation is our dynamical law, presenting an evolution equation in the "internal time" a which means that the evolution of possible matter fields is measured with respect to the expansion or contraction of the universe. Concerning the singularity problem there is no real progress because the equation cannot tell us about anything happening beyond the singularity at $a = 0$.

The issue of initial conditions now appears in a different light: we have to choose an initial value for the wave function $\psi(a)$ at some a_0 (we only need one value to fix one of the two parameters of the general solution; the other one would be fixed by normalization). At $a = 0$, corresponding to the classical singularity, the differential equation is still singular, but we can try to cancel the divergence by requiring the initial condition $\psi(0) = 0$. This is DeWitt's initial condition [1], and it seems that we do have a relation between this initial condition and the dynamical law since it was motivated by a regularity condition.

Unfortunately, this is not true since the uniqueness of this condition depends on the matter content as well as the factor ordering. Even worse, however, is the fact that in a more complicated system DeWitt's initial condition would not be well-posed: the only solution satisfying it would vanish identically.

There are attempts [2] to make DeWitt's condition well-posed in general by adding a "Planck potential" to the Wheeler–DeWitt equation solely for the purpose of creating one (and only one) solution which decreases toward zero at $a = 0$ such that it can be hand-picked by the initial condition. This presents another attempt to link the dynamical law with the initial condition, but the introduction of the Planck potential and the choice of the wave function remain artificial.

Later, DeWitt's condition has been replaced by alternative proposals which originate from different motivations, most importantly the tunneling proposal of Vilenkin's [3] and the no-boundary proposal of Hartle and Hawking's [4]. They are not directly related to the dynamical law, however, and they do not solve the singularity problem.

Was the hope originating in the stability of the quantized Hydrogen atom misleading? Do we have to accept the cosmological singularity and the fact that we still have to choose our initial conditions even for a whole universe? Maybe surprisingly, the answer is not a certain Yes. For we have used only simple quantum mechanics to derive the quantum model, while a full quantum theory of gravity in this spirit exists only formally and a precise link is lacking. The full theory would be much more complicated and it would have to fulfill many consistency conditions which can easily be missed in a simple model with only a single gravitational degree of freedom, a. There is in fact one indication that the quantization we used is not correct: while the Planck length $l_{\rm P}$ does appear in the Wheeler–DeWitt equation (2), there is no realization of discreteness of space as we would have expected (a can still take arbitrary continuous values).

The situation has changed over the last decade since we now have a mathematically well-defined candidate for quantum gravity (loop quantum gravity/quantum geometry [5, 6]) from which we can derive quantum cosmological models (see [7] and references therein). There are many consistency conditions to fulfill which leads to a theory very different from the Wheeler–DeWitt quantization; in particular, they imply that space is in fact discrete. For our model we need the following information: The wave function ψ_n is now only defined at integer values n related to a by $a_n^2 = \frac{1}{6}l_{\rm P}^2|n|$ rather than on a continuous line, and the total volume of space can only take discrete values

$$V_n = (\tfrac{1}{6}l_{\rm P}^2)^{\frac{3}{2}}\sqrt{(|n|-1)|n|(|n|+1)}\,. \qquad (3)$$

Here the Planck length appears and sets the scale for the discreteness and the smallest non-zero volume $V_{\rm min} = \frac{1}{6}l_{\rm P}^3$.

Over the last few years, the cosmological sector of quantum geometry, loop quantum cosmology, has been studied. A first observation is that we have a well-defined, *finite* operator which quantizes the classically divergent a^{-1} [8]. This operator has eigenvalues

$$(a^{-1})_n = 16 l_{\rm P}^{-4}\left(\sqrt{V_{n+1}} - \sqrt{V_{n-1}}\right)^2 \qquad (4)$$

in terms of (3), which have the upper bound (for $n = 2$)

$$(a^{-1})_{\max} = \frac{32(2-\sqrt{2})}{3l_{\rm P}} \,. \tag{5}$$

Now we can see that also the second indication we got from the Hydrogen atom is realized: The classical divergence of a^{-1} is cut off by quantum effects leading to an upper bound, which diverges in the classical limit $l_{\rm P} \to 0$ owing to the appearance of the Planck length in the denominator. Another surprising result is that $(a^{-1})_0 = 0$, i.e. the inverse radius of the universe vanishes at the classical singularity $n = 0$ where also the radius itself vanishes. This classically counterintuitive but well-understood fact will be of importance later.

Thus, both facets of the Hydrogen atom are also present in our new quantum cosmological model. To finally settle the singularity issue, however, we still have to face the acid test: whether or not we can extend the evolution to something "beyond the singularity". For this we need the dynamical law, the loop quantization of the Friedmann equation. It turns out to be [9]

$$(V_{n+2} - V_n)\psi_{n+1} - 2(V_{n+1} - V_{n-1})\psi_n + (V_n - V_{n-2})\psi_{n-1} = -\tfrac{1}{3}8\pi G l_{\rm P}^2\, \hat{H}(n)\, \psi_n \tag{6}$$

where we use the volume eigenvalues (3) and a matter Hamiltonian $\hat{H}(n)$. It looks very different from the Wheeler–DeWitt equation (2), most obviously because it is a difference rather than a differential equation. This is a direct consequence of the discreteness of space and also time, which is now given by the label n instead of the continuous a. Nevertheless, it is straightforward to check, using a Taylor expansion, that the Wheeler–DeWitt equation approximates our discrete equation at large volume $n \gg 1$. When the volume is small, however, there are large discrepancies between the discrete and the continuous formulation which lead to qualitative changes. This is right where a modified evolution is needed since we have seen that the Wheeler–DeWitt formulation cannot deal with the singularity problem.

To check for a singularity we try to follow the evolution as long as possible, starting with initial values for ψ_n at two times n_0 and $n_0 - 1$ and evolving backward toward the classical singularity at $n = 0$. This is possible as long as the lowest coefficient, $V_n - V_{n-2}$ in the difference equation is non-zero. At first one can anticipate a problem because this coefficient is zero if (and only if) $n = 1$ such that we are not able to compute ψ_0, the wave function at the classical singularity, in this way. This time, however, we are safe: While we cannot find this value, we do not even need it since it decouples completely from the evolution equation. Let us ignore this value and try to continue the evolution, computing ψ_{-1} using (6) with $n = 0$. Now two terms containing the unknown ψ_0 appear, but both of them drop out. The first one, is $2(V_{n+1} - V_{n-1})\psi_n$, which is zero for $n = 0$. We also have $\frac{1}{3}8\pi G l_{\rm P}^2\, \hat{H}(n)\, \psi_n$ being zero for $n = 0$, but more subtly so: each term in the matter Hamiltonian, the kinetic and the potential term, contains either components of the metric or the inverse metric, reducing to a or a^{-1} in the isotropic context. Classically, one would be zero and the other infinite at the classical singularity, but we have seen that in loop quantum cosmology *both* have to be zero at the classical singularity. Thus, $\hat{H}(0) = 0$ and ψ_0

completely drops out of the evolution equation; ψ_{-1} is completely determined by ψ_1 which we know in terms of our initial data. In the same way, we can now follow the evolution completely determining all values of the wave function for positive and negative n. The evolution does not stop at $n = 0$ which, consequently, does not represent a singularity anymore.

In this analysis the point $n = 0$ was special because some coefficients of the difference equation vanish. However, it does not represent a singularity or a "beginning" of the universe. Instead, we can determine what happens at the other side, represented by negative n, by using our evolution equation. Intuitively, there is a collapsing branch of the universe at negative times $n < 0$ which collapses down to a single point, bounces and enters our expanding branch. Furthermore, one can show that the sign of n is the orientation of space such that the universe "turns its inside out" at $n = 0$.

Without $n = 0$ representing a beginning, it is not so natural to impose initial conditions there; and it is not even possible because ψ_0 drops out of the evolution equation. Still, this point plays an important role for the issue of initial conditions [10], the main interest of this essay. Let us take a closer look at what we discussed before: Starting with initial values at n_0 and $n_0 - 1$ we evolved backward until we reached $n = 0$ and continued beyond the singularity. At $n = 0$ we noticed that we could not determine ψ_0, which we just ignored because ψ_0 decoupled completely. However, the part of the evolution equation which was supposed to give us ψ_0 — with $n = 1$ in (6) — still has to be satisfied, resulting in a linear equation for ψ_1 and ψ_2. Those two values, in turn, are linear functions of our two initial values ψ_{n_0} and ψ_{n_0-1}. Therefore, the dynamical law gives us one linear condition for the two initial values, which is just what we need to fix the wave function uniquely up to its norm.

Thus, for the first time we can now see an intimate link between the dynamical law and initial conditions as part of the law. The discrete structure, the solution of the singularity problem and the issue of initial conditions are all related in a way which is very special to the case of gravity and cosmology, for it is the Planck length which allows the discreteness of space and the classical singularity problem which makes the point $n = 0$ special.

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